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# Contents

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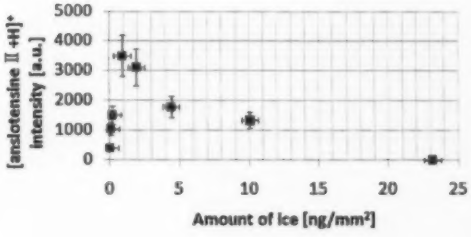
**Enhancing peptide molecular imaging by depositing ice in time-of-flight secondary ion mass spectrometry**

Naofumi Aoki, Manabu Komatsu, Masafumi Kyogaku, Hiroyuki Hashimoto

● We brought out a quantitative relationship between ionization enhancement and the amounts of the adherent ice on the sample. ● Ice deposition method is suitable for mass imaging analysis because the original distribution of the sample constituents is maintained. ● The adherent ice behaves as an additional source of protons and enhances the detection intensity of the sample in TOF-SIMS measurement.

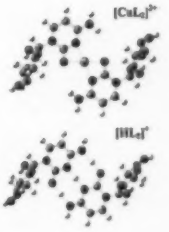



*5–11*

**Structure and stability of electronsprayed cytidine$_n$Cu$^{2+}$ and cytidine$_n$H$^+$ ($n$ = 1–4) compounds in the gas phase**

Shuqin Zhang, Junguo Dong, Li Xu, Ping Cheng, Zhen Zhou, Jiamo Fu

● The stability and structure of $[CuL_n]^{2+}$ and $[L_nH]^+$ (L = cytidine) were investigated. ● The main interaction between the Cu(II) and L for $[CuL_n]^{2+}$ is coordination. ● The main interaction between Ls for $[L_nH]^+$ is hydrogen bond. ● The stability order for $[CuL_n]^{2+}$ is $[CuL_2]^{2+}$ > $[CuL]^{2+}$ > $[CuL_4]^{2+}$ > $[CuL_3]^{2+}$. ● The stability order for $[L_nH]^+$ is $[L_2H]^+$ > $[LH]^+$ > $[L_3H]^+$ > $[L_4H]^+$.

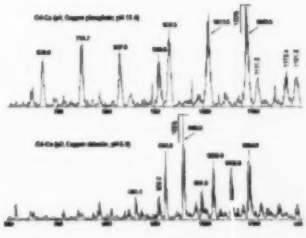



*12–22*

**ESI-MS study of self-assembly-formed tetraglycine macrocyclic ligand complex of Cu(II)**

Manuela Murariu

● Copper–tetraglycine (Cu–$G_4$) complexes were characterized by ESI-MS at various pH and Cu:$G_4$ molarratios. ● $G_4$ mobilizes a large amount of copper ions from insoluble salts on increasing pH. ● Increased pH and copper ions induce oligomerization of $G_4$.



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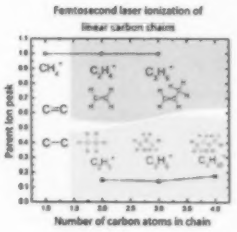
http://dx.doi.org/10.1016/S1387-3806(13)00326-6

*23–26*

**Product ion distribution from the femtosecond laser irradiation of small acyclic hydrocarbon molecules**

A.A. Zaidi, A. Hu, J.H. Sanderson, W.W. Duley

● This paper discusses small organic hydrocarbon chain molecules in intense laser fields. ● Laser molecular ionization and time of flight mass spectrometry has been used in experimentation. ● Experimental findings show that parent ion peaks are stronger in alkene chains than corresponding alkane chains. ● In linear chain hydrocarbon molecules stability with respect to femtosecond laser field increases by introduction of a carbon–carbon double bond.

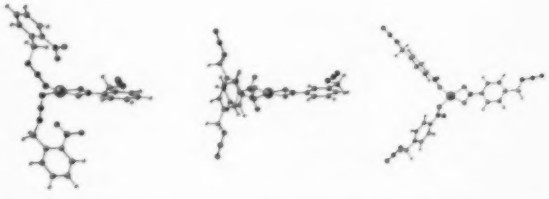



*27–36*

**Gas-phase interaction between nickel (II) and nitrobenzyl azides: An ESI-MS$^n$ study**

Bárbara M.P. Cunha, Inês N. Trindade, Narciso A.S. Couto, P.J. Costa, P. Rodrigues, M.T. Barros, M.L. Costa, M.F. Duarte, M.T. Fernandez, Paulo J. Amorim Madeira

● Organoazide interaction with metals. ● Metal complexation as isomer probe in ESI-MS. ● Density functional calculations in mass spectrometry problems.

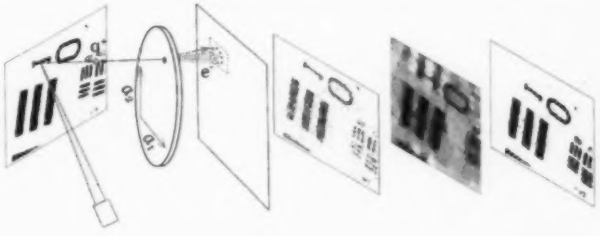



*37–46*

**Sparse spectral techniques for emission imaging**

Andrei Kharchenko, Julia H. Jungmann, Luke MacAleese, Ron M.A. Heeren

● Data analysis strategy for "blurred" imaging data sets acquired with image intensifiers, like microchannel plates. ● High-resolution of the original image is retrieved with a significant degree of sparseness. ● Optimum amount of information is recovered from a sparse emission data set. ● Predict the least-time consuming experimental approach by determination of minimal frame requirement.

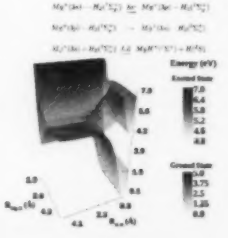


*47–55*

**$Mg^+(^2S)$ and $Mg^+(^2P)$ in reaction with $H_2(^1\Sigma_g^+)$: A description of the energy surfaces explaining the mechanisms**

M. Satta, M. Marquéz-Mijares, E. Yurtsever, S. Bovino, F.A. Gianturco

● Ion molecule reaction guided by non adiabatic transitions. ● Intermediate complex formation with hydrogen triplet state. ● Exothermic product channels with $MgH^+$ formation. ● Ab initio potential energy surfaces. ● Non adiabatic Landau–Zener dynamics at crossing.

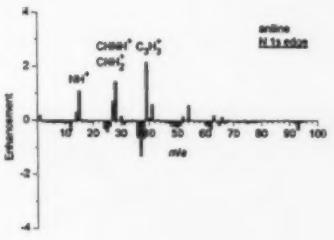


***56–60***

**Specific fragmentation of the K-shell excited/ionized aniline molecule studied by electron impact**

Kazumasa Okada, Yasuhiko Kashiwagi, Masamichi Sakai

● Fragmentation of aniline upon K-shell excitation/ionization was studied. ● Main fragments were assigned with an isotopologue and by the MLR analysis. ● The $C_3H_3^+$ was a characteristic fragment ion at the N 1s edge. ● The aniline molecular cation can isomerize prior to dissociation.

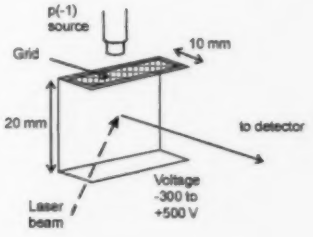



***61–68***

**Laser-mass spectrometry study of ultra-dense protium p(−1) with variable time-of-flight energy and flight length**

Leif Holmlid

● The laser-TOF-MS target used for the condensed material p(-1), ensuring that a condensed superfluid phase is observed.

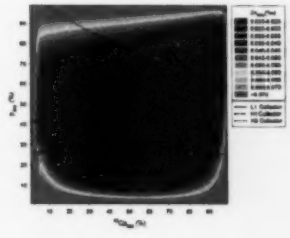



***69–75***

**Precise analysis of Ca isotope ratios ($\delta^{44/40}$Ca) using an optimized $^{43}$Ca–$^{42}$Ca double-spike MC-TIMS method**

G.O. Lehn, A.D. Jacobson, C. Holmden

● Monte Carlo error model used to optimize a $^{43}$Ca–$^{42}$Ca double-spike MC-TIMS method. ● Double-spike parameters selected to improve precision and limit collector damage. ● Optimization tested by analyzing Ca isotope standard reference materials ($n$ = 171). ● External precision improved by two- to ten-fold over previous double-spike methods.

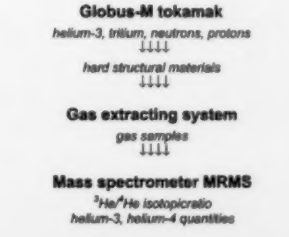


***76–80***

**Mass-spectrometric measurements of helium isotopes in structural materials of the Globus-M tokamak**

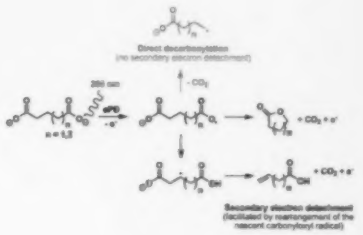
N.N. Aruev, B.S. Boltenkov, A.N. Novokhatsky

● Helium-3 and tritium are generated by deuterium plasma of tokamak. ● These gases diffuse into the bulk of structural materials of plant. ● Gases extracted from hard samples are analyzed by means of mass spectrometer. ● Quantities of helium isotopes and their ratios are determined. ● These values give a possibility to estimate the rate of generation of $^{3}$He and $^{3}$T.



**81–94**

**Characterisation of the ionic products arising from electron photodetachment of simple dicarboxylate dianions**

Benjamin B. Kirk, Adam J. Trevitt, Berwyck L.J. Poad, Stephen J. Blanksby

● We measure ionic photodetachment products arising from simple dicarboxylate dianions. ● Major products arise from decarboxylation of the nascent carbonyloxyl radical. ● Decarboxylation results in formation of a distonic radical anion. ● Rearrangement of the carbonyloxyl radical facilitates secondary electron detachment. ● These secondary electron detachment pathways compete kinetically with decarboxylation.